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Investigation of coal entrained-flow gasification in O₂-CO₂ mixtures for oxy-fuel IGCC

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Abstract. Purpose of the study is to obtain fundamental knowledge about Kuznetsk bituminous coal entrained-flow gasification in O₂-CO₂ mixtures for oxy-fuel IGCC. To achieve this purpose, it is necessary to carry out experimental and numerical studies. To obtain universal knowledge, "CKTI" single-stage gasifier with fuel consumption of 5-15 kg/h was chosen as an experimental installation. In order to identify the most interesting and informative experimental regimes, a number of computational studies have been carried out, whose results are given in the paper. A numerical (CFD) model has been developed, which includes all the submodels necessary for the study. Two series of numerical calculations were carried out. In the first series, the composition of the blast (O₂ = 0-100%, CO₂ = 0-100%) and the oxygen ratio were varied at constant consumption of coal and blast. In the second series, the composition of the blast (O₂ = 0-100%, CO₂ = 0-100%) and the coal consumption were varied at constant oxygen ratio and blast flow rate. The study allowed predicting and analyzing the temperature distribution and the syngas components content along the gasifier height with different CO₂ concentrations in the blast.

1. Introduction

The technology of integrated gasification combined cycle (IGCC) allows to use cheapest and most common fuel - coal for production of electrical energy with efficiency of more than 50% [1]. However, modern environmental requirements for energy technologies are compelling to remove from exhaust gases not only harmful substances, such as nitrogen oxides, sulfur, etc., but also greenhouse gas CO₂. This requires the application of CO₂ capture technologies (carbon capture and storage, CCS), which reduce the efficiency by about 10% [2].

Fundamentally, CCS IGCC technologies are divided into three groups: pre-combustion (CO capture from syngas before combustion, which reduces CO₂ formation), post-combustion (CO₂ capture from combustion products of synthesis gas), and oxy-fuel (compression and disposal of all combustion products, including CO₂). The most effective technology is oxy-fuel, which allows reducing emissions of exhaust gases to the atmosphere while maintaining relatively high efficiency of more than 40% [2]. The development of oxy-fuel IGCC requires the operation of equipment in a new mode. The gasifier in the oxy-fuel IGCC cycle being developed by the UrFU, will use blast O₂-CO₂ mixture instead of air or oxygen, and CO₂ as a transporting agent - instead of nitrogen.

A number of research teams involved in the development of the Japanese oxy-fuel IGCC [2] conducted experimental studies and calculations (computational fluid dynamics, CFD) [3, 4] on the adaptation of a two-stage air-blown entrained-flow gasifier such as Mitsubishi Heavy Industries (MHI) to operate on O₂-CO₂ mixture. In the experimental and calculation study [3], the operation of pilot



two-stage gasifier with coal consumption of 100 kg/h, oxygen ratio of 0.49-0.55, blast composition: $O_2 = 25-30\%$, $CO_2 = 0-70\%$, $N_2 = 0-75\%$ is considered. In numerical study [4], industrial two-stage gasifier with coal consumption of 70 t/h, oxygen ratio of 0.4-0.45, blast composition: $O_2 = 25-45\%$, $CO_2 = 0-75\%$, $N_2 = 0-75\%$ is simulated. Firstly, in both studies, the ranges of operating parameters are rather limited, which is explained in the first case [3] by the technical capabilities of the experimental gasifier, and in the second [4] – by requirements (maximum efficiency) to the industrial gasifier. Secondly, both works consider two-stage gasifiers, whose operation principle is quite specific. All this makes it difficult to obtain fundamental knowledge about the coal gasification process in the O_2 - CO_2 mixtures.

Purpose of the present study is to obtain fundamental knowledge about Kuznetsk bituminous coal entrained-flow gasification in O_2 - CO_2 mixtures for oxy-fuel IGCC.

To achieve this purpose, it is necessary to carry out experimental and numerical studies. To obtain universal knowledge, CKTI single-stage gasifier [5] with fuel consumption of 5-15 kg/h was chosen as an experimental installation. In order to identify the most interesting and informative experimental regimes, a number of computational studies have been carried out, whose results are given in the paper.

Research objectives:

1) developing CFD-model to investigate the entrained-flow gasification of Kuznetsk coal of grade D in O_2 - CO_2 mixtures;

2) carrying out two calculation series: the first - with varying blast composition ($O_2 = 0-100\%$, $CO_2 = 0-100\%$) and oxygen ratio at constant coal and blast flow rate; and the second - with varying blast composition ($O_2 = 0-100\%$, $CO_2 = 0-100\%$) and coal flow rate at constant oxygen ratio and blast flow rate;

3) identifying gasifier optimum operating conditions and developing recommendations for conducting experimental studies.

2. Simulation method

Numerical simulation is performed using the method of computational fluid dynamics (CFD), which is widely used in solving such problems [3-5]. The basic submodels of CFD-modeling include the following equations: continuity, energy, components transport, forces balance for discrete phase, the momentum conservation law, etc. The number of calculated trajectories of the coal particles is 2000. The adherence condition is satisfied on the gasifier walls. The temperature was set constant over the entire gasifier wall surface. As calculation algorithm, fully coupled solver is chosen, in which the velocity and pressure in the calculation element are determined simultaneously. For each calculation, 10000-20000 iterations are required. The maximum value of the root-mean-square residual is 0.0001. Unbalance in terms of variables does not exceed 1%.

The choice of the optimal turbulence model depends on the flow type, the required accuracy of the solution, the available computational resources, and so on. It is believed that the standard k- ϵ model satisfies for simulating free jets. Earlier [6], this model was verified by solving similar problem.

To describe the processes of coal particle motion, the Lagrange method is used. With this approach, the particle motion is described by the equations of the material point dynamics, taking into account the resistance and gravity forces. The use of this method is justified by the low volume particles concentration, on the order of 10^{-4} - 10^{-5} m³/m³, at which there is no need to simulate the interaction between particles, that considerably complicates calculations.

To reduce the calculation time, it was assumed that the evaporation of the coal moisture takes place instantaneously. The rate of volatile substances release was described by single-stage model. Taking into account the high rates of gas-phase reactions with volatile substances, their composition was assumed to be equilibrium, which is quite acceptable for estimating calculations. To calculate the rates of combustion (1), Boudouard (2) and steam gasification (3) reactions, the diffusion-kinetic model is used. Kinetic constants of Kuznetsk coal of grade D, previously [5] obtained by thermogravimetric analysis (TGA), were used. A more detailed description of all the submodels is given in [7].



To simulate homogeneous reactions (4-7), the combined Eddy Dissipation / Finite Rate Chemistry model was used. According to the mechanism of this model, the minimum reaction rate calculated using Finite Rate Chemistry and Eddy Dissipation schemes is the real reaction rate.



The geometry of the CKTI gasifier has beam symmetry due to the 8 oxidizer outlet holes in the burner nozzle. That is why a 45° segment was chosen to model the gasifier (Fig. 1). This allowed optimizing the computational process and reducing the calculation time. As a result of mesh analysis, it is established that the optimal number of mesh elements is 250000.

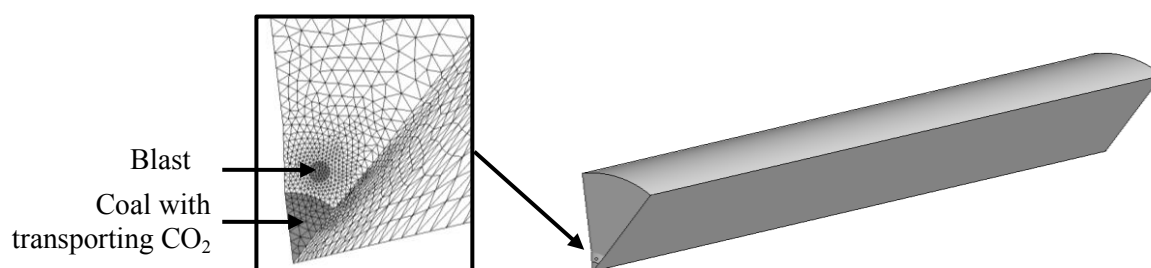


Figure 1. Modelling segment.

3. Results and discussion

The gasifier operation parameters at which the simulation is performed are shown in Table 1.

Table 1. Modelling gasifier operation parameters

Parameters	Series 1	Series 2
Oxygen ratio	0-0.8	0.8
Coal flow rate, kg/h	12	0-12
Coal grade	Kuznetsk bituminous coal of mark D	
Blast composition, %	$\text{O}_2 = 0-100\%$; $\text{CO}_2 = 0-100\%$	
Blast flow rate, kg/h	18	
Blast temperature, °C	522	
Transporting agent	CO_2	
Transporting agent flow rate, kg/h	1.512	
Transporting agent and coal temperature, °C	25	
Wall temperature, °C	1300	
Gasifier pressure, MPa	0.132	

The distribution of temperature and volume percentages of the syngas components along gasifier dimensionless height are shown in Fig. 2.

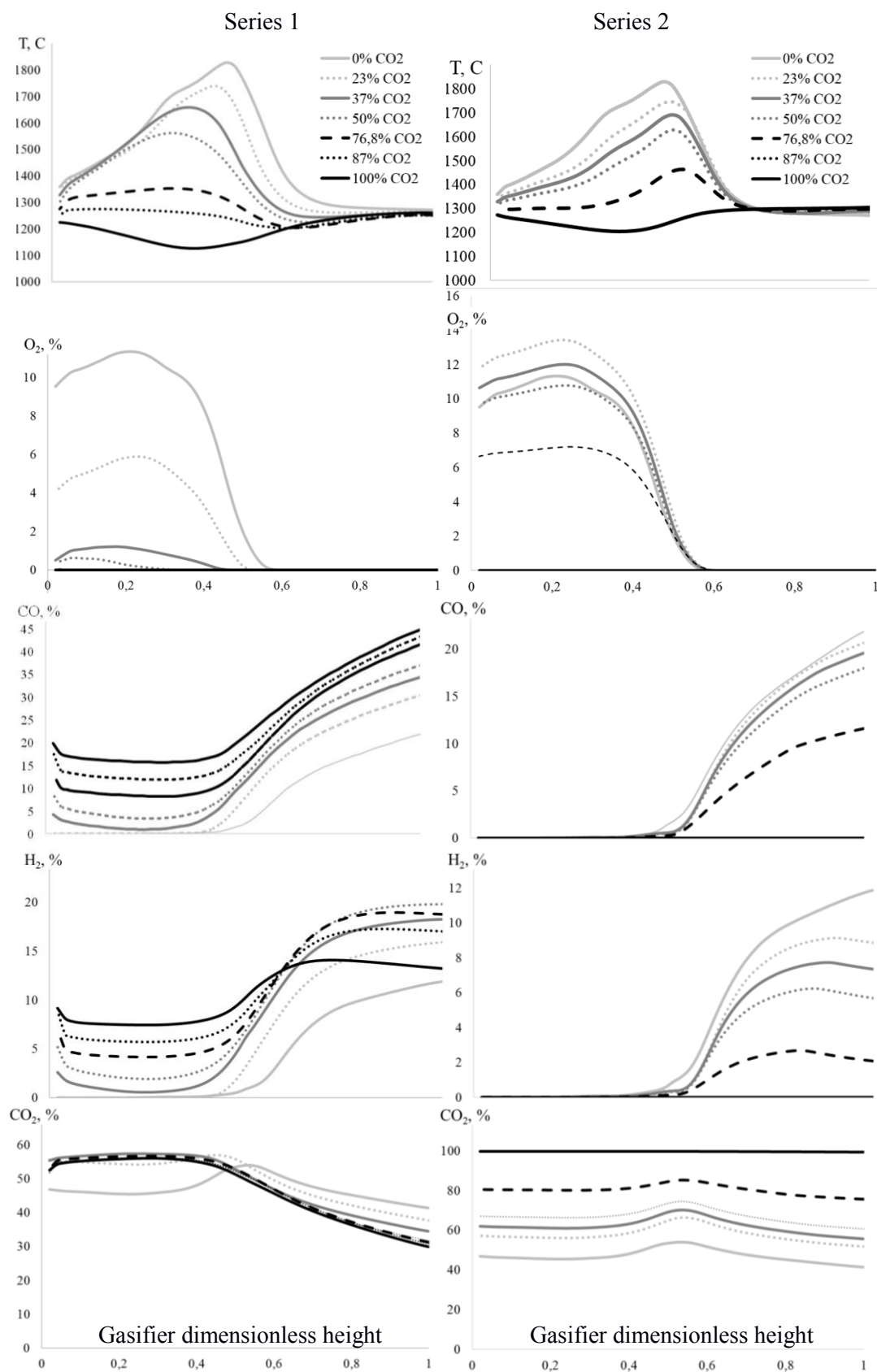


Figure 2. Distribution of average cross-sectional variables along the gasifier dimensionless height.

In series 1, where the blast CO_2 concentration is increased, the peak and average temperatures decrease, and the flame moves toward the burner (Figure 2). It is explained by decrease of exothermic reactions rate (combustion) and growth of endothermic one (Boudouard). At blast CO_2 concentration of more than 87%, the temperature peak associated with the exothermic reactions practically disappears. But temperature peak in outlet from the gasifier arises, caused by syngas heating by gasifier wall (1300°C). Autothermal mode of the gasifier operation is only partially possible with a CO_2 concentration in the blast below 80%, otherwise the syngas temperature at the gasifier height is below the wall temperature. In series 2, as in series 1, when the blast CO_2 concentration increases, the peak temperatures decrease, but the flame moves away from the burner because less fuel releases, less heat and the combustion process is delayed.

The syngas oxygen content is expected to decrease with increasing blast CO_2 concentration. In series 1 at CO_2 concentration of more than 50%, oxygen is practically absent from the entire height of the gasifier, since the oxygen ratio is extremely low. In series 2 with constant oxygen ratio, oxygen is absent in the gasifier only at 100% CO_2 in the blast, and in all other cases it is consumed approximately to the middle of the gasifier, after which a reduction zone begins in which endothermic gasification reactions occur.

In series 1, the volumetric concentration of CO is expected to increase with increasing of blast CO_2 concentration due to reduction of oxygen ratio. The peak at the exit from the gasifier indicates that the gasifier generates syngas with composition far from that corresponding to chemical equilibrium. In series 2, CO concentration has the opposite tendency - it decreases with increasing of blast CO_2 concentration, since at the same oxygen ratio the gasification rate is determined by the temperature, which decreases with increasing share of the blast CO_2 concentration.

In series 1, the nature of the hydrogen concentration change in the gasifier height first half is explained by the water gas shift reaction: at low CO concentration and high CO_2 , hydrogen is reduced. In the second half of the gasifier height, the hydrogen concentration starts manifesting multidirectional effect on the other components concentration, so the maximum hydrogen concentration at the gasifier outlet is characterized by the regime with the blast CO_2 concentration of 50%. In series 2, the nature of the hydrogen concentration change is similar to that of CO, and is explained by the same reasons.

In series 1 with CO_2 in the blast below 23%, the syngas CO_2 volumetric concentration has pronounced peak at the middle of the gasifier height due to the prevalence of the combustion reaction over the Boudouard reaction. The same peak is observed in series 2 with blast CO_2 concentration less than 100%. In series 1, the syngas CO_2 concentration is reduced at the gasifier outlet with increase of the blast CO_2 concentration, since with less oxygen the less CO_2 is formed in the syngas. The reverse picture in series 2 - with an increase of the blast CO_2 concentration CO_2 at the gasifier output is increasing due to constant oxygen ratio.

4. Conclusion

In consequence of the work conducted, the following tasks were accomplished:

1) Numerical (CFD) model has been developed that includes all the submodels necessary to study the entrained-flow coal gasification in the O_2 - CO_2 mixtures in the CKTI gasifier.

2) Two series of numerical calculations were carried out. In the first series, the composition of the blast ($\text{O}_2 = 0$ -100%, $\text{CO}_2 = 0$ -100%) and the oxygen ratio were varied with constant consumption of coal and blast. In the second series, the composition of the blast ($\text{O}_2 = 0$ -100%, $\text{CO}_2 = 0$ -100%) and the coal consumption were varied with constant oxygen ratio and blast flow rate. The study allowed predicting and analyzing the temperature distribution and the syngas components content along the gasifier height with different CO_2 concentrations in the blast.

3) Analysis of the numerical study results made it possible to establish that in both series:

a) at blast CO_2 concentration more than 80%, the unit goes into the allothermal operation mode, which in the experiment course can lead to reaction space cooling down and chemical reactions rates decrease;

b) the syngas components concentrations do not reach their chemical equilibrium values at given temperature and pressure in the gasifier outlet. It suggests that this fact must be taken into account in the thermodynamic analysis of the gasifier operation;

c) in order to increase the process autothermicity level and to approximate the syngas composition to the chemical equilibrium state, it is necessary to maintain the oxygen ratio above the theoretically necessary one.

In the further research, series of experiments will be conducted on the CKTI entrained-flow coal gasification in O_2 - CO_2 mixtures, taking into account the results of this numerical study.

References

- [1] Ryzhkov A, Bogatova T, Gordeev S 2018 *Fuel* **214** 63-72
- [2] Oki Y, Hamada H, Kobayashi M, Yuri I, Hara S 2017 *Energy Procedia* **114** 501-4
- [3] Watanabe H, Tanno K, Umetsu H, Umemoto S 2015 *Fuel* **142** 250-9
- [4] Watanabe H, Ahn S, Tanno K 2017 *Energy* **118** 181-9
- [5] Abaimov N A, Osipov P V and Ryzhkov A F 2016 *J. of Phys.: Conf. Series* **754** 112001
- [6] Chernetskiy M Y, Kuznetsov V A, Dekterev A A, Abaimov N A and Ryzhkov A F 2016 *Thermophysics and aeromechanics* **23** 615-26
- [7] Abaimov N A and Ryzhkov A F 2015 *Thermal Engineering* **62** 767-72